Quarter-filled honeycomb lattice with a quantized Hall conductance

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We study a generic two-dimensional hopping model on a honeycomb lattice with strong spin-orbit coupling, *without the requirement that the half-filled lattice be a topological insulator*. For quarter-(or three-quarter) filling, we show that a state with a quantized Hall conductance generically arises in the presence of a Zeeman field of sufficient strength. We discuss the influence of Hubbard interactions and argue that spontaneous ferromagnetism (which breaks time reversal) will occur, leading to a quantized anomalous Hall effect.

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Topological insulators (TIs) are a new state of matter with a bulk gap but protected edge/surface modes.[1] Quantum Hall states[3] are examples of time-reversal violating TIs. Recently, time-reversal-invariant TIs have been predicted[1] and seen in experiments.[2] They are characterized by a nontrivial Z_2 index in the bulk, and the presence of chiral edge/surface states which are robust against localization due to static disorder.

One of the simplest models of two-dimensional TIs is the Kane-Mele model,[4] which is a tight-binding model on a honeycomb lattice with hopping and spin-orbit interactions. A more realistic model is given by a monolayer of the three-dimensional TI alkali iridate A_2IrO_3 (where $A = Na$, Li), where the various tight-binding hopping parameters are known from a fit to *ab initio* calculations.[5] We will be working with a generic model on a honeycomb lattice which has no symmetries other than lattice translations, $2\pi/3$ rotations, and time reversal. Since there are two sublattices and two spins, a generic tight-binding model has four bands. Here and henceforth, when we talk about quarter or three-quarter filling, we will mean either one or three of these four bands, respectively, are filled.

Our goal is to construct an experimentally realizable system with a quantized anomalous Hall effect (AHE).[6] The AHE has historically described the effect of magnetic order (spontaneous or otherwise) on the Hall conductance. We will describe a proposal for observing a quantized Hall conductance in the absence of a perpendicular magnetic flux which could be realized, for example, in a monolayer of alkali iridate doped to three-quarter filling, and subject to a Zeeman field perpendicular to the monolayer. Previous proposals in this direction[7] have also either explicitly violated time reversal, or appealed to spontaneous magnetic order in interacting TIs. Our proposal does require strong spin-orbit couplings but does not require the material to be a TI at half filling.

Generic models we consider share the following properties: They are defined on a honeycomb lattice with two sites per unit cell. Including spin, there are four bands. In the Brillouin zone (BZ) shown in Fig. 1 there are two kinds of special points. The Γ and M points are time-reversal invariant (modulo a reciprocal lattice vector), while the K and K' points go into each other under time reversal. Time-reversal symmetry forces the bands to be degenerate at the Γ and M_α points. In a simple spin-independent nearest-neighbor-only tight-binding model (e.g., graphene) there are van Hove singularities at Γ and M_α, whereas there are Dirac cones at K and K'. Neither of these features is generic under the addition of time-reversal-invariant spin-orbit couplings: The Dirac cones at the K and K' points can be gapped by either a $L_z S_z$-type spin-orbit coupling, or by a sublattice antisymmetric potential,[4] while the van Hove singularities are converted into Dirac cones by a Rashba coupling. Figure 2 shows such a generic time-reversal-invariant band structure.

We begin with a noninteracting model with threefold rotational and time-reversal symmetry, and focus on the generic Dirac crossings at the Γ and M_α points. Now consider a Zeeman field in the Z direction (perpendicular to the monolayer). This preserves the threefold rotational symmetry of the lattice, but breaks time reversal and will therefore provide a mass gap to the Dirac points at Γ and M_α. We know that if the variation of a parameter in the Hamiltonian leads to the touching of two bands at a Dirac point for some critical value, a Chern number of ± 1 must be exchanged between the two bands[8] as the parameter passes through that value.[8] By the lattice rotational symmetry all M_α must have the same exchange of Chern number. Since there are three M points and a single Γ point, it is clear that the Chern number exchange must be either ± 2 or ± 4. This means that upon reversing the Zeeman coupling, the Chern number of the lowest band must reverse, implying that its Chern number is either ± 1 or ± 2. Of course, the Zeeman coupling should be strong enough to create a hard gap (the bands should not overlap in energy) in order to form an insulator. We will show that in a simple model of A_2IrO_3 with Hubbard interactions, such a hard gap may form spontaneously.

While the result is completely generic, we illustrate it in the specific model of Ref. 5, in which the noninteracting Hamiltonian for a freestanding monolayer of sodium/lithium iridate is[5]

$$H_{SI} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.}) + \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \hat{t}_{ij} c_j, \tag{1}$$

where the spin indices have been suppressed, $\langle ij \rangle$ is a sum over nearest neighbors, $\langle\langle ij \rangle\rangle$ is a sum over next-nearest neighbors, and the matrix $\hat{t}_{ij}$ in spin space is

$$\hat{t}_{ij} = t_0' + i t' \sigma_a. \tag{2}$$

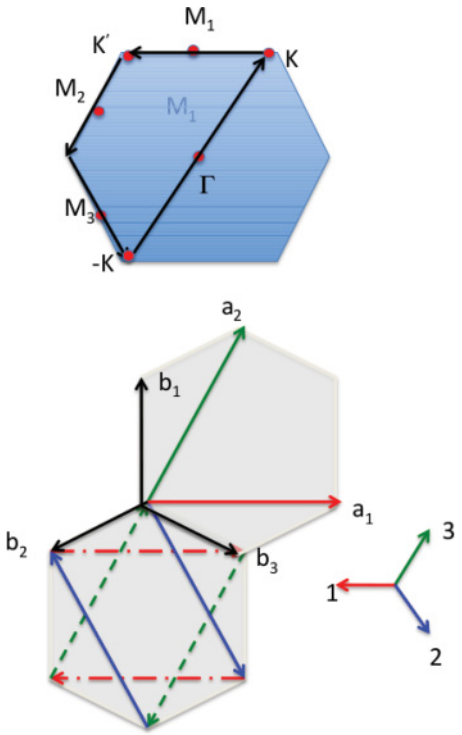

FIG. 1. (Color online) Top: The Brillouin zone of the honeycomb lattice. The Γ and three M points are time-reversal invariant, while the K and K' points go into each other under time reversal. The arrows show the path along which the band structure will be plotted. Bottom: The next-nearest neighbor hops in A_2IrO_3 are shown by dot-dashed red lines that go with σ_1, the solid blue lines that go with σ_2, and the dashed green lines that go with σ_3. The primitive lattice vectors are $\vec{a}_1$ and $\vec{a}_2$, while $\vec{b}_1,\vec{b}_2,\vec{b}_3$ are nearest-neighbor hopping vectors. The auxiliary triad shows the projection of the original crystal axes onto the plane of the honeycomb lattice. Note that these directions match the nearest-neighbor hops and the labels of the associated σ matrices.

This hopping term is diagonal in the sublattice. Referring to Fig. 1, the hopping is antisymmetric in the sublattice index (A,B). Further, each hop comes with a σ_a matrix, the index a corresponding to the projection of the original crystal axes onto the 111 plane. Thus, hopping along the primitive lattice vector $\pm\vec{a}_1$ carries a σ_1, hopping along the vector $\pm(\vec{a}_1-\vec{a}_2)$ carries a σ_2, and hopping along $\pm\vec{a}_2$ carries a σ_3. Let us denote the Pauli matrices in the sublattice space by τ_a. We obtain

$$h_{\rm SI}(\vec{k}) = t_0' F_0(\vec{k}) - t[f_r(\vec{k})\tau_1 - f_i(\vec{k})\tau_2] - t'\tau_3[\vec{F}(\vec{k})\cdot\vec{\sigma}], \tag{3}$$

where

$$f(\vec{k}) = f_r + if_i = e^{i\vec{k}\cdot\vec{b}_1} + e^{i\vec{k}\cdot\vec{b}_2} + e^{i\vec{k}\cdot\vec{b}_3}, \tag{4}$$

$$F_0(\vec{k}) = \cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos[\vec{k}\cdot(\vec{a}_2-\vec{a}_1)], \tag{5}$$

$$F_1(\vec{k}) = \sin(\vec{k}\cdot\vec{a}_1), \tag{6}$$

$$F_2(\vec{k}) = \sin[\vec{k}\cdot(\vec{a}_2-\vec{a}_1)], \tag{7}$$

$$F_3(\vec{k}) = -\sin(\vec{k}\cdot\vec{a}_2). \tag{8}$$

The parameters for the 111 plane of Ir in Na_2IrO_3 are estimated[5] as $t = 310$ K, $t_0' = -130$ K, and $t' = 100$ K.

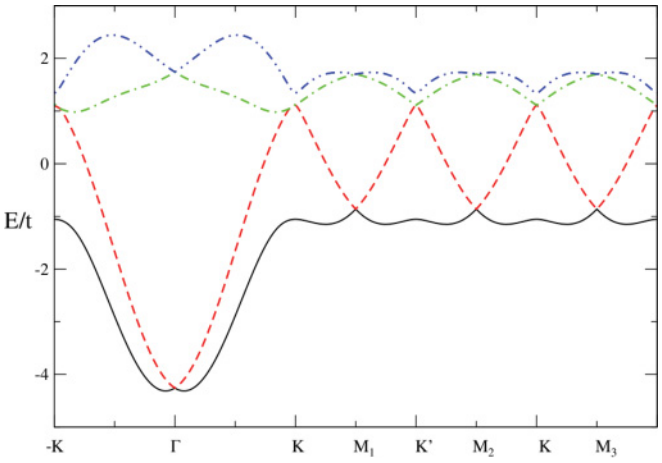

FIG. 2. (Color online) The band structure for a monolayer of A_2IrO_3 with the addition of a Rashba term with $\lambda_R = 0.4t$. The path in the BZ followed is shown in Fig. 1. The generic Dirac crossings at the Γ and M_α points can be seen.

One first diagonalizes $\vec{F}\cdot\vec{\sigma}$, which has eigenvalues $\pm|\vec{F}|$, and obtains the energies at $\vec{k}$ as

$$E_\pm(\vec{k}) = t_0' F_0(\vec{k}) \pm \sqrt{t^2|f|^2 + t'^2|\vec{F}|^2}. \tag{9}$$

It is seen that the four bands come in two pairs, degenerate at all momenta. This is the result of inversion symmetry and clearly not generic. For a monolayer on a substrate, a Rashba spin-orbit coupling arising from the substrate $\vec{E}$ field perpendicular to the 111 plane is induced. A nearest-neighbor Rashba coupling leads to an additional term

$$h_R(\vec{k}) = i\lambda_R\vec{G}(\vec{k})\cdot\boldsymbol{\sigma}\tau_+ - i\lambda_R\vec{G}^*(\vec{k})\cdot\boldsymbol{\sigma}\tau_-, \tag{10}$$

where

$$G_1(\vec{k}) = \sqrt{\frac{2}{3}}\left(e^{i\vec{k}\cdot\vec{b}_1} - \frac{1}{2}e^{i\vec{k}\cdot\vec{b}_2} - \frac{1}{2}e^{i\vec{k}\cdot\vec{b}_3}\right) \tag{11}$$

with cyclic permutations of $\vec{b}_1,\vec{b}_2,\vec{b}_3$ defining G_2,G_3.

Due to its special symmetries, this model does not show generic behavior for $\lambda_R < t'$. For this parameter range, in addition to the usual Dirac points at Γ, and M_α there are also Dirac points at K,K'. For $t' > t_*'$ (where t_*' is a function of λ_R, but tends to $3t/8$ as $\lambda_R \to 0$) the M points are unsplit. However, for $\lambda_R < t' < t_*'$, each M point splits into three Dirac points lying on the zone boundary. The central point is still at M and the other two "satellites" are symmetrically distributed about it. At the special point $\lambda_R = t'$, the satellites coalesce with the Dirac points at K,K'. For $\lambda_R > t'$ the would-be Dirac points at K,K' are gapped, and the only Dirac points left are the generic ones. In the following we will focus on this case.

A typical band structure including $\lambda_R = 0.4t$ (satisfying $\lambda_R > t'$) is shown in Fig. 2. One clearly sees the Dirac-like crossings at the Γ and M_α points.

For weak Zeeman coupling, a gap will open at the Dirac points, but the two bands will overlap in energy (at different momenta), and the system will be metallic at quarter or three-quarter filling [recall that this means that one or three of the four bands described by Eq. (1) is full]. Increasing the Zeeman coupling will lead to a hard gap and thus a quantized

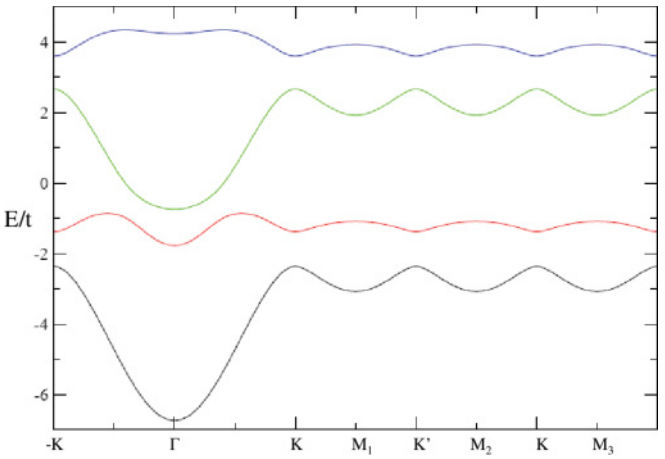

FIG. 3. (Color online) The Hartree-Fock band structure at $U = 10t$ and three-quarter filling in A_2IrO_3 with $\lambda_R = 0.1t$. The path followed in the BZ is shown in Fig. 1. Note the hard gap and the flatness of the topmost empty band (blue online).

Hall conductance. For the noninteracting model, the critical Zeeman field is $0.37t$. A calculation shows that the Chern number for these parameters is -1. We note parenthetically, that even for the nongeneric case $\lambda_R < t'$ the Chern number of the highest energy band is nonzero (1), but different from the above. Once a hard gap has been established, the Chern number is robust against arbitrary deformations of the Hamiltonian which do not close the gap. In particular, one could softly break the lattice rotational symmetry, add a Kane-Mele-type spin-orbit coupling or a staggered sublattice potential, and also tilt the Zeeman away from the perpendicular to the monolayer.

Let us now consider the influence of interactions. It is known that a strong enough Hubbard U leads to an antiferromagnet in the half-filled TI.[9] An on-site Hubbard interaction (typically of size $\frac{U}{t} \simeq 10$) spontaneously breaks time-reversal symmetry at three-quarter filling in the Hartree-Fock approximation. Assuming only that lattice translation symmetry is intact but allowing for the possibility of rotational and sublattice symmetry breaking, we find in Hartree-Fock that the magnetization is in the Z direction (perpendicular to the monolayer), and the gap is strongly enhanced. Because there is no spin-rotation symmetry in this model, the Z direction is the natural one, and the order parameter is Ising-like. This implies that the spin waves are fully gapped, and that there should be a finite-temperature phase transition even in the two-dimensional material.

Of course, it could happen that the system chooses to break lattice translation symmetry by forming a larger unit cell, as happens in graphene at a quarter doping.[10] However, in graphene, this is a result of nongeneric features such as Fermi-surface nesting, which is sensitive to the details of the band structure, and is not generic (there are also other competing states in graphene at quarter filling). Furthermore, a strong enough Zeeman field in the Z direction will make our lattice symmetric solution energetically favorable. We will leave a further discussion of the issue of other possible ground states at quarter (or three-quarter) filling[11] to future work.

We now speculate on the effects of long-range (1/r) Coulomb interactions in this system, which can coexist with the Hubbard interaction. Long-range Coulomb interactions will be present because the material is insulating, and will likely suppress charge density wave states, which are one avenue of translation symmetry breaking. Secondly, since the band has a nonzero Chern number we expect skyrmionic excitations[12] to be the lowest energy charged excitations in some regime of parameters. Finally, because the empty band is relatively flat, it may represent an environment in which analogs of fractional quantum Hall states will be stable when the band is partially occupied.[13,14]

Let us briefly consider the potential effects of disorder. In analogy with the integer quantum Hall effect, we expect that disorder will localize most states, except those near the band center, which carry the Hall conductance. In a recent study,[15] this expectation has been numerically confirmed in the disordered Kane-Mele model with Zeeman fields. So the quantized anomalous Hall effect should become easier to observe in a disordered system.

One can ask whether other simple lattices can support similar states under generic conditions, where the only Dirac points are those mandated by time-reversal symmetry. The simplest square lattice two-band model does not support such states. The reason has to do with the fact that the BZ has only two M points. Repeating the argument above Eq. (1), we see that the Chern number exchange is ± 1 or ± 3, implying that the states have Chern number $\pm\frac{1}{2}$ or $\pm\frac{3}{2}$, which is impossible for a two-dimensional band insulator. The half-filled triangular lattice with one band per unit cell would have a tendency to become antiferromagnetic when interacting. Thus the honeycomb lattice seems to be the simplest one in which the desired properties can be realized.

In summary, we have shown that given a generic one-body Hamiltonian on a honeycomb lattice that has time-reversal symmetry, $2\pi/3$ lattice rotational symmetry, and strong spin-orbit coupling, one can obtain a band with nonzero Chern number at quarter- or three-quarter filling, with strong enough Rashba coupling, and an external Zeeman coupling. The result is completely general and does not depend on specific features such as Fermi surface nesting, van Hove singularities, inversion symmetry, etc. Since the system does not even have to be a TI at half filling, this increases the range of possible material realizations. One potentially promising material is A_2IrO_3 with $A =$ Na, Li, with the Chern number of the three-quarter-filled system being ± 1. In the bulk it is half filled and antiferromagnetically ordered[16] below $T_N = 15$ K. A monolayer of the 111 Ir plane sandwiched by two layers of Na would induce three-quarter doping,[17] where we expect it to become a ferromagnetic quantized anomalous Hall insulator with an Ising-like order parameter in the presence of Hubbard interactions of realistic strength. It may be quite difficult to grow a single monolayer doped in the manner described, but possibly the surface layer of a thin enough film will display the same properties. We intend to investigate this in future work.

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